1,3-diphenylpropane-1,2-diol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 149 °C

Global applicability domain: Inside

Local applicability domain index: 6.34e-01

Confidence level: 5.63e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
4,4'-Propane-2,2-diylbis(2-tert-butylphenol)	[1,1'-Biphenyl]-4,4'-diol, 3,3',5,5'-tetramethyl-	3,3'-Dimethylbisphenol A
Measured: 114	**Measured:** 222	**Measured:** 139
Predicted: 117	**Predicted:** 188	**Predicted:** 157